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DEPARTMENT OF MATHEMATICS

UNIVERSITY OF HOUSTON

HOUSTON, TEXAS

NASA CR-

147520

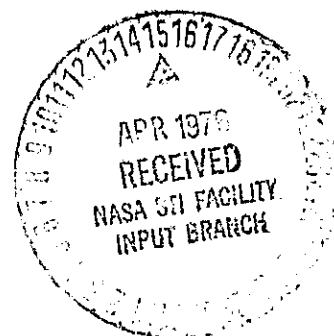
(NASA-CR-147520) UHML: PROGRAM
DESCRIPTION USER GUIDE (Houston Univ.) 21 p
HC \$3.50 CACL 09B

N76-20861

Unclass

G3/61 21496

UHML:
PROGRAM DESCRIPTION
BY W. A. COBERLY &
C. R. WIGINTON
REPORT #48 OCTOBER 1975



PREPARED FOR
EARTH OBSERVATION DIVISION, NASA
UNDER
CONTRACT NAS-9-12777

HOUSTON, TEXAS 77004

*UHMLE - Program Description
User Guide*

October, 1975

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Report #48

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I. Introduction

This program computes maximum-likelihood estimates for the general normal mixture. That is, MLE estimates are found for $\alpha_k, \mu_k, \Sigma_k, k=1, \dots, M$ in the model

$$p(x) = \sum_{k=1}^M \alpha_k p_k(x; \mu_k, \Sigma_k)$$

where $\{p_k\}$ are multivariate (N-dimensional) normal density functions with means μ_k and covariance Σ_k , and $\{\alpha_k\}$ are the mixing proportions. The algorithm used is described in detail in [1]. Simply stated, it consists of solving the following fixed point equations. For $\epsilon_\alpha, \epsilon_\mu, \epsilon_\Sigma$ arbitrary positive constraints less than two (called iteration weights), find at each iteration new parameter values (indicated by primes) using previous values (without primes) from the following system of equations. For a sample of LTOT observation vectors x_1, \dots, x_{LTOT} the iteration equations are

$$\alpha'_k = (1 - \epsilon_\alpha) \alpha_k + \epsilon_\alpha \left\{ \frac{\alpha_k}{LTOT} \sum_{j=1}^{LTOT} \frac{p_k(x_j)}{p(x_j)} \right\}$$

$$\mu'_k = (1 - \epsilon_\mu) \mu_k + \epsilon_\mu \left\{ \frac{1}{LTOT} \sum_{j=1}^{LTOT} x_j \frac{p_k(x_j)}{p(x_j)} \right\}$$

$$\Sigma'_k = (1 - \epsilon_\Sigma) \Sigma_k + \epsilon_\Sigma \left\{ \frac{1}{LTOT} \sum_{j=1}^{LTOT} (x_j - \mu_k)(x_j - \mu_k)^T \frac{p_k(x_j)}{p(x_j)} \right\}$$

for $k = 1, \dots, M$.

The data vectors must be read onto a direct access device, prior to execution of UHMLE. The data is stored sequentially by vector (pixel) in any format, specified by the reader.

The number of data vectors in core is flexible. Hence only L (possibly $L = 1$) vectors at a time may be read into core, in order to minimize the program size, or all data vectors may be stored in core, in order to eliminate I/O time. An intermediate choice is usually called for in large data sets.

The program allows the user to fix any subsets of the mixture parameters (e.g. hold the Σ 's constants while iterating on the α 's and μ 's, etc). This fixed set may be redefined at various times in the iteration process (i.e. when the α 's and μ 's converge for fixed Σ , then fix μ 's and iterate on α 's and Σ 's). The Σ 's may be assumed to be diagonal or full symmetric covariance matrices. There is considerable time saved in computing the likelihoods if the diagonal form is specified. Hence in the early iterations the diagonal assumption might be used, changing over to the full covariance mode later in the iteration process for a more refined solution. This flexibility allows the user to choose the sequence of parameter configurations in the iteration process which he feels will optimize the computation time required as well as possibly avoid convergence to suboptimal local maxima of the likelihood function.

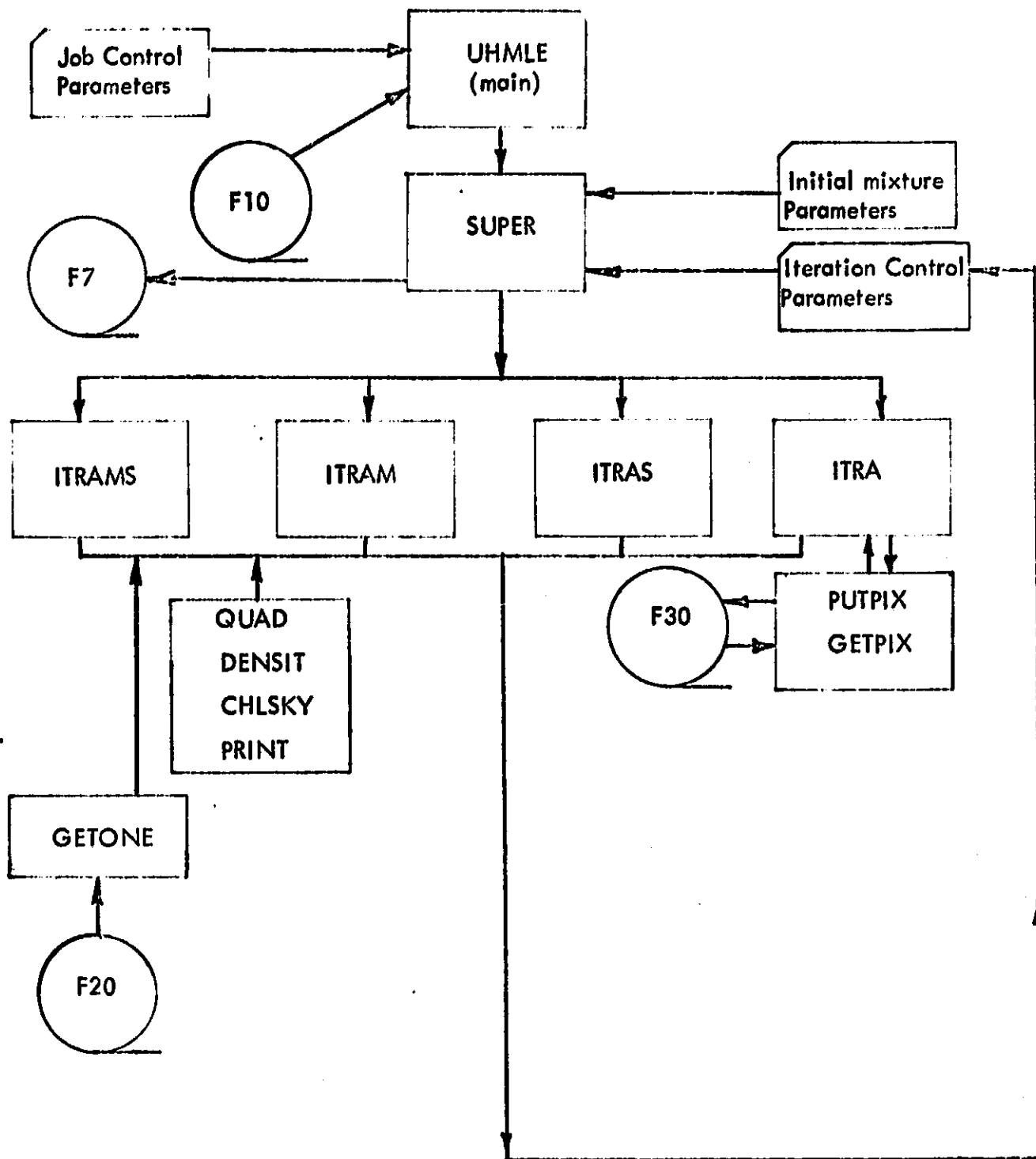
References

- [1] B. C. Peters and H. Walker - An Iterative Procedure for Obtaining Maximum-Likelihood Estimates of the Parameters for a Mixture of Normal Distributions. July, 1975
- [2] B. C. Peters and H. Walker - Addendum to "An Iterative Procedure for Obtaining Maximum-Likelihood Estimates of the Parameters for a Mixture of Normal Distributions". September, 1975

II. PROGRAM ELEMENTS

- MLO2 - Main driver. Reads job control parameters and sets up data arrays.
- SUPER - Reads initial values for mixture parameters. Reads successive sets of iteration control parameters and supervises the iteration method prescribed.
- ITRAMS - Computes updated values for α, μ, Σ for each iteration. (α may be fixed.)
- ITRAM - Computes updated values for α, μ , for each iteration with Σ fixed. (α may be fixed).
- ITRAS - Computes updated values for α, Σ , for each iteration with μ fixed. (α may be fixed).
- ITRA - Computes updated values for α for each iteration with μ, Σ fixed. In this case the component likelihoods are computed only once and stored on disk in a temporary data set.
- QUAD - Computes the quadratic forms for either full or diagonal covariances.
- PRINT - Prints appropriate results at each iteration.
- CHSLKY - Computes the inverse covariance matrix and determinant by the Cholesky decomposition method.
- GETONE - Monitors transfer of data from disk to core. This activity is transparent to the ITR prefixed routines.
- PUTPIX - Monitors storage of the component likelihoods onto disk. Used by ITRA only.
- GETPIX - Monitors retrieval of the component likelihoods from disk. Used by ITRA only.
- DENSIT - Computes the posterior probability for all classes for each observation (pixel).

UHMLE FLOW DIAGRAM



III. VARIABLE DESCRIPTIONS

1. Job Control Parameters

- N - Number of channels (dimension of measurement space).
- M - Number of classes
- L - Number of observation vectors in core at one time.
- N2 - $N(N+1)/2$
- NN - N^2
- NL - $N \times L$
- ML - $M \times L$
- LTOT - Total number observations vectors in the data set.
- RUNID - A four character run identification code.
- F7 - Fortran unit number for output signatures.
- F10 - Fortran unit number for input of LTOT.
- F20 - Fortran unit number for direct access file containing data vectors.
- F30 - Fortran unit number for direct access temporary file containing component likelihoods.
- ICORE - Upper limit for the dimension (single precision words) of the blank common work data array.
- FMT(18)- Format for the input data vectors read by GETONE.
- The values of F7, F10, F20, F30 are presently set to 11, 12, 13, 14 respectively. In order to alter these, change cards UHML1480-510.
 - Presently N must be 30 or less and M must be 20 or less. L is limited by ICORE. To change these limitations, the Common/ITRWRK/ must be altered in each routine.
 - Presently ICORE < 16000. To change this, alter cards UHML1450-60 and UHML2010.
 - $ICORE = M(6+4N + 3N^2 + L) + N(6N+L)$

2. Iteration Control Parameters

IFLAGA	- 1	means to iterate on alpha.
	0	means to hold alpha fixed.
IFLAGM	- 1	means to iterate on means.
	0	means to hold the means fixed.
JFLAGS	- 1	means to iterate on the sigmas.
	0	means to hold the sigmas fixed.
MODES	- 1	general symmetric covariance.
	2	diagonal covariance.
ITLIM	-	maximum number of iterations allowed for this iteration phase.
TOLA	-	convergence tolerance for ALPHA
TOLM	-	convergence tolerance fo MU
TOLS	-	convergence tolerance for SIGMA
EPSA	-	iteration weight for ALPHA
EPSM	-	iteration weight for MU
EPSS	-	iteration wleight for SIGMA
ITRPNT	-	1 means to print results at each step of the iteration.

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9

ALPH(K) CURRENT VALUE OF PROPORTION ESTIMATE FOR KTH CLASS
 ALPHO(K) LAST ("O" IS FOR OLD) VALUE OF PROPORTION ESTIMATE FOR KTH CLASS

INDM INDEX FOR VECTOR OF LENGTH $M \times N$ CONSISTING OF M MEAN VECTORS OF LENGTH N SIDE-BY-SIDE

MU(INDM) CURRENT VALUE OF COMPONENT OF THE "LONG" MEAN VECTOR
 MUC(INDM) LAST VALUE OF COMPONENT OF THE "LONG" MEAN VECTOR

INDS INDEX FOR VECTOR OF LENGTH $M \times N^2$ CONSISTING OF M "LOWER TRIANGULAR HALVES" OF $N \times N$ COVARIANCE MATRICES
 EACH ONE OF THESE M IS INDEXED IN THE FOLLOWING ORDER

1
 2 3
 4 5 6
 7 8 9 10

 N^2

SIG(INDS) CURRENT VALUE OF A COMPONENT OF THE "LONG" CO-VARIANCE MATRIX
 SIGO(INDS) LAST VALUE OF A COMPONENT OF THE "LONG" COVARIANCE MATRIX
 INCSS INDEX FOR SIGIN
 SIGIA(INCSS) CURRENT VALUE OF A COMPONENT OF THE INVERSE OF A COVARIANCE MATRIX INDEXED IN THE SAME WAY AS THE COVARIANCE MATRIX. FOR THIS INVERSE WE HAVE MULTIPLIED THE DIAGONAL ELEMENTS BY ONE HALF FOR EFFICIENCY OF LATER COMPUTATIONS.

PIX(K) KTH COMPONENT DENSITY FUNCTION
 P MIXTURE DENSITY FUNCTION
 R RATIO OF COMPONENT DENSITY TO MIXTURE DENSITY

X(K) KTH COMPONENT OF OBSERVATION VECTOR
 XM(K) KTH COMPONENT OF OBSERVATION VECTOR MINUS KTH COMPONENT OF CLASS MEAN VECTOR

XBUFF $N \times L$ BUFFER ARRAY OF OBSERVATIONS...DATA IN CORE AT ONE TIME
 PXBUFF $M \times L$ BUFFER ARRAY OF LIKELIHOOD (ONLY USED BY ITRA)
 XLP $N \times N$ TRIANGULAR FACTOR FROM SUBROUTINE CHLSKY
 XTEMP $N \times N$ WORK MATRIX FROM SUBROUTINE CHLSKY
 CFI $N \times N$ INVERSE MATRIX PRODUCED BY SUBROUTINE CHLSKY
 RECALL WE MULTIPLY DIAGONAL ELEMENTS BY 1/2

EPSA ITERATION WEIGHT FOR ALPHA
 EPSM ITERATION WEIGHT FOR MU
 EPSS ITERATION WEIGHT FOR SIGMA
 Q ONE-HALF VALUE OF QUADRATIC FORM COMPUTATION

CALFLC CONTROL FLAG FOR CALLING SUBROUTINE GETONE
 DELA SUP OVER ALL CLASSES OF $|ALPH(K) - ALPHO(K)|$
 DELM SUP OVER ALL CLASSES OF SUP OVER ALL COORDINATES OF $|ML(K) - MLC(K)|$
 DELS SUP OVER ALL CLASSES OF SUP OVER ALL I & J OF THE

IPT POINTER IN GET/PUT ROUTINES

ITRCT COUNTER FOR NUMBER OF ITERATIONS

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IV. FILE DESCRIPTIONS

1. F10 - LTOT Unit, fortran unit 12.

This file contains only one data field, LTOT the number of observation vectors in the intermediate image data set residing on unit F20. This is a one record file with format (18,72x). LTOT is usually computed from tape to disk in a prior job step. If fortran unit 5 is assigned to F10 then this must be the first card in the data input stream.

2. F20 - Intermediate image data set, fortran unit 13.

This file contains the observation vectors (pixels) formatted according to FMT. This data set should reside on a direct access device (disk) since this file is rewound at each iteration (except when iterating on α only in ITRA). The data set may contain any number of channels. A subset may be selected by specifying the format FMT. The file is accessed in the GETONE routine. Each logical record is an N-dimensional vector or pixel

<u>Rec</u>	<u>Pixel</u>
1	Channel 1, Channel 2;..., Channel N
2	Channel 1, Channel 2,..., Channel N
.	
.	
.	
LTOT	Channel 1, Channel 2,..., Channel N
-EOF-	

3. F30 - Temporary likelihoods data set, fortran unit number 14.

This unit is accessed only in ITRA, i.e., when IFLAGM = IFLAGS = 0. The likelihoods for each class are computed and stored for each pixel on the 1st iteration of ITRA through the PUTPIX routine. The logical record format is

20A4. (This may be changed to binary). This file is accessed by GETPIX on subsequent iterations of ITRA.

4. F7 - Output signature data set, fortran unit 11.

This file contains the UHMLE signatures. They may be punched on cards or stored on disk for latter access.

V. Input Data Streams.

The input data stream, typically the card reader (fortran unit 5), consists of the following card images. All input parameter cards ignore the first 10 columns (except FMT). This allows comments or labels to be used. The deck setup is as follows:

1. Job control parameters

<u>Parameter</u>	<u>Format</u>
RUNID	(10x,A4)
M	(10x,I10)
N	"
L	"
FMT	(18A4)

2. Initial values of the mixture parameters

	ALPHA	(10x,7F10.4)
1st Class	* MUØ	(10x,7F10.4)
	SIG	"
Mth Class	* MUØ	(10x,7F10.4)
	SIG	"

* each mean vector or covariance matrix must begin on a new card.

3. Iteration Control Parameters*

IFLAGA	(10x,I10)
IFLAGM	"
IFLAGS	"
MØDES	"
ITLIM	"
TØLA	(10x,F10.0)
TØLM	"
TØLS	"
EPSA	"
EPSM	"
EPSS	"
ITRPNT	(10x,I10)

*The iteration control block may be repeated as often as desired.

VI. Sample Deck Setup

The following is a sample job deck designed for use on the IBM OS/360 system. The first iteration phase iterates on the mean vectors only, assuring a fixed diagonal covariance and fixed equal proportions. This iteration configuration is used until the TOLM tolerance or ITLIM requirement is met. Then the second set of iteration parameters are read in and all mixture parameters (full covariance) are estimated. In the third iteration phase the μ 's and Σ 's are held fixed and only the α 's are varied.

```
//UHMLE JOB
// EXEC FORTHCLG
//SYSIN DD *
```

```
<
< INSERT THE UHMLE SOURCE DECK HERE >
< >
```

```
/*
//GO,FT11F001 DD SYSOUT=B
//GO,FT12F001 DD DSN=88F10,UNIT=SYSUA,DISP=(OLD,PASS),SPACE=(TRK,1),
// DCB=(RECFM=F,LRECL=80)
//GO,FT13F001 DD DSN=88F20,UNIT=SYSUA,DISP=(OLD,PASS),SPACE=(CYL,5),
// DCB=(RECFM=FB,LRECL=80,BLKSIZE=7200)
//GO,FT14F001 DD DSN=88F30,UNIT=SYSUA,DISP=(NEW,PASS),SPACE=(CYL,5),
// DCB=(RECFM=FB,LRECL=80,BLKSIZE=7200)
//GO,SYSIN DD *
```

```
<
< JOB CONTROL PARAMETER CARDS FOLLOW >
< >
```

```
RUNID TEST
M 5
N 4
L 1000
(48X,4F4,0)
```

```
<
< INITIAL VALUES OF MIXTURE PARAMETERS FOLLOW >
< >
```

ALPHO	.2	.2	.2	.2	.2		
MU W1	19.27	17.11	29.24	34.39			
SIG	2.48	3.27	5.40	0.68	1.02	1.54	-1.11
	-1.85	1.02	3.31				
MUD F1	25.53	26.51	28.41	27.48			
SIG F1	1.04	.94	2.02	.13	.04	1.07	.17
SIG	.28	.64	.95				
MUD B1	24.23	24.73	32.57	34.45			
SIG B1	5.93	10.61	20.44	.99	1.68	1.46	-2.69
SIG	-5.83	.85	4.62				
MUD S1	22.68	24.56	24.35	23.61			
SIG S1	.76	.57	1.25	.46	.43	1.18	.50
SIG	.54	1.02	1.54				
MUD G2	21.94	20.35	25.29	26.18			
SIG G2	.64	.36	1.08	.04	.22	.63	.01
SIG	.25	.49	1.11				

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< ITERATION CONTROL PARAMETER SET 1 FOLLOWS >

IFLAGA 0
 IFLAGM 1
 IFLAGS 0
 MODES 2
 ITLIM 10
 TOLA 0.0
 TOLM .5
 TOLS 0.0
 EPSA 1.
 EPSM 1.
 EPSS 1.
 ITRPNT 0

< ITERATION CONTROL PARAMETER SET 2 FOLLOWS >

IFLAGA 1
 IFLAGM 1
 IFLAGS 1
 MODES 1
 ITLIM 10
 TOLA .05
 TOLM .1
 TOLS .5
 EPSA 1.
 EPSM 1.
 EPSS 1.
 ITRPNT 0

< ITERATION CONTROL PARAMETER SET 3 FOLLOWS >

IFLAGA 1
 IFLAGM 0
 IFLAGS 0
 MODES 1
 ITLIM 10
 TOLA .0005
 TOLM 0.0
 TOLS 0.0
 EPSA 1.
 EPSM 1.
 EPSS 1.
 ITRPNT 1

//

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VII. SAMPLE RUN OUTPUT

```

RUNID  TEST
M      =      5
N      =      4
L      =    1000
LTOT   =    1000
FMT    = (48X,4F4.0)
ICORE  IS      9507
    
```

JOB CONTROL PARAMETERS

```

*****
ITERATION NUMBER  0  RUN ID  TEST
    
```

INITIAL VALUES OF MIXTURE PARAMETERS

ITERATION	ALPHA	MU	SIG	SIG	SIG	SIG
1	.2000	.2000	.2000	.2000	.2000	.2000
2		19,2700	17,1100	29,2400	34,3900	
3		2,4800	3,2700	5,4000		
4		.6800	1,0200	1,5400		
5		-1,1100	-1,8500	1,0200	3,3100	
6		25,5300	28,5100	28,4100	27,4800	
7		1,0400				
8		.9400	2,0200			
9		.1300	.0400	1,0700		
10		.1700	.2800	.6400	.9500	
11		24,2300	24,7300	32,5700	34,4500	
12		5,9300				
13		10,6100	20,9400			
14		.9900	1,6800	1,4800		
15		-2,6900	-5,8300	.8500	4,6200	
16		22,6800	24,5600	24,3500	23,6100	
17		.7600				
18		.5700	1,2600			
19		.4600	.4300	1,1800		
20		.5000	.5400	1,0200	1,5900	
21		21,9400	20,3500	25,9900	26,1800	
22		.6400				
23		.3600	1,0800			
24		.0400	.2200	.6300		
25		.0100	.2500	.4900	1,1100	

```

DELA = .00000000D 00
DELM = .00000000D 00
DELS = .00000000D 00
    
```

FIRST ITERATION PHASE

```

=====
=====
IFLAGA =      0
IFLAGM =      1
IFLAGS =      0
MODES  =      2
ITLIN  =     10
TOLA   =      ,0000
TOLM   =      ,5000
TOLS   =      ,0000
EPSA   =     1,0000
EPSM   =     1,0000
EPSS   =     1,0000
ITRPNT =      0

```

```

*****
ITERATION NUMBER      RUN ID  TEST

```

1	MU	17,8031	16,5129	27,1694	31,3981
2	MU	23,7707	27,0716	28,6527	28,1058
3	MU	22,6907	24,8613	30,0646	31,1144
4	MU	21,0216	23,3486	23,3769	22,8112
5	MU	19,2719	18,2692	22,8665	23,8401
DELM =		,33356190 01			

```

*****
ITERATION NUMBER      5      RUN ID  TEST

```

1	MU	16,6778	14,8320	26,2050	31,1280
2	MU	22,5021	25,2806	25,3615	24,7759
3	MU	21,3214	22,2943	29,1891	30,9607
4	MU	19,8427	21,8596	21,8481	21,2645
5	MU	19,1461	18,0818	22,5252	23,4409
DELM =		,48255680 00			

SECOND ITERATION PHASE

```

=====
I FLAGA =      1
I FLAGM =      1
I FLAGS =      1
MODES  =      1
ITLIM  =     10
TOLA   =     ,0500
TOLM   =     ,1000
TOLS   =     ,5000
EPSA   =     1,0000
EPSM   =     1,0000
EPSS   =     1,0000
ITRPNT =      0
=====

```

```

*****
ITERATION NUMBER      1      RUN ID  'TEST'

```

	ALPHA	,2108	,2002	,1886	,2012	,1991
1	MU	16,6639	14,8111	26,2000	31,1372	
	SIG	2,1491				
	SIG	2,5256	4,3368			
	SIG	,5766	,6716	1,5796		
	SIG	-,6004	-1,3074	,9739	2,7428	
2	MU	22,4559	25,2242	25,2934	24,7135	
	SIG	,8719				
	SIG	,7195	1,5809			
	SIG	,1527	,0281	1,0942		
	SIG	,1525	,1841	,6034	,9720	
3	MU	21,3160	22,2876	29,1754	30,9450	
	SIG	4,0012				
	SIG	6,8823	13,5315			
	SIG	,5259	,7899	1,1029		
	SIG	-2,0998	-4,3828	,6186	3,4737	
4	MU	19,7642	21,7195	21,7747	21,1898	
	SIG	,6325				
	SIG	,3791	1,1063			
	SIG	,3202	,3385	,9569		
	SIG	,4302	,3833	,8357	1,4568	
5	MU	19,1452	18,0087	22,5618	23,5316	
	SIG	,5810				
	SIG	,2315	,9248			
	SIG	,0632	,1602	,5755		
	SIG	,0203	,1329	,4628	,9817	
DELA =		,11360460	01			
DELM =		,14010480	00			
DELS =		,74084760	01			

ITERATION NUMBER 4 RUN ID 'TEST'

ALPHA	,2061	,2010	,1931	,1992	,2006
1					
MU	16,7034	14,9441	26,1353	31,0450	
SIG	2,3907				
SIG	2,9303	4,8791			
SIG	,6370	,9129	1,4492		
SIG	,7009	-1,3608	,8310	2,7143	
2					
MU	22,4471	25,2265	25,2865	24,6933	
SIG	,9040				
SIG	,7286	1,5571			
SIG	,1751	,0284	1,1312		
SIG	,1915	,2184	,6583	1,0322	
3					
MU	21,1581	21,9598	29,1732	31,0526	
SIG	4,5883				
SIG	8,1097	16,0966			
SIG	,6068	,9891	1,0574		
SIG	-2,4166	-4,9941	,4798	3,4870	
4					
MU	19,7524	21,7273	21,7716	21,1802	
SIG	,6253				
SIG	,3892	1,0121			
SIG	,3259	,3293	,9537		
SIG	,4392	,4231	,8480	1,4683	
5					
MU	19,1637	18,0153	22,5616	23,5397	
SIG	,6039				
SIG	,2613	,9172			
SIG	,0578	,1689	,5851		
SIG	,0143	,1715	,4705	,9680	

DELA = ,1020178D+02
DELM = ,5515645D+01
DELS = ,3150645D 00

=====

IFLAGA = 1
IFLAGM = 0
IFLAGS = 0
MODES = 1
ITLIM = 10
TOLA = ,0005
TOLM = ,0000
TOLS = ,0000
EPSA = 1,0000
EPSM = 1,0000
EPSS = 1,0000
ITRPNT = 1

THIRD ITERATION PHASE

ITERATION NUMBER 1 RUN ID 'TEST'

ALPHA ,2053 ,2012 ,1936 ,1990 ,2006
DELA = ,7867705D+03

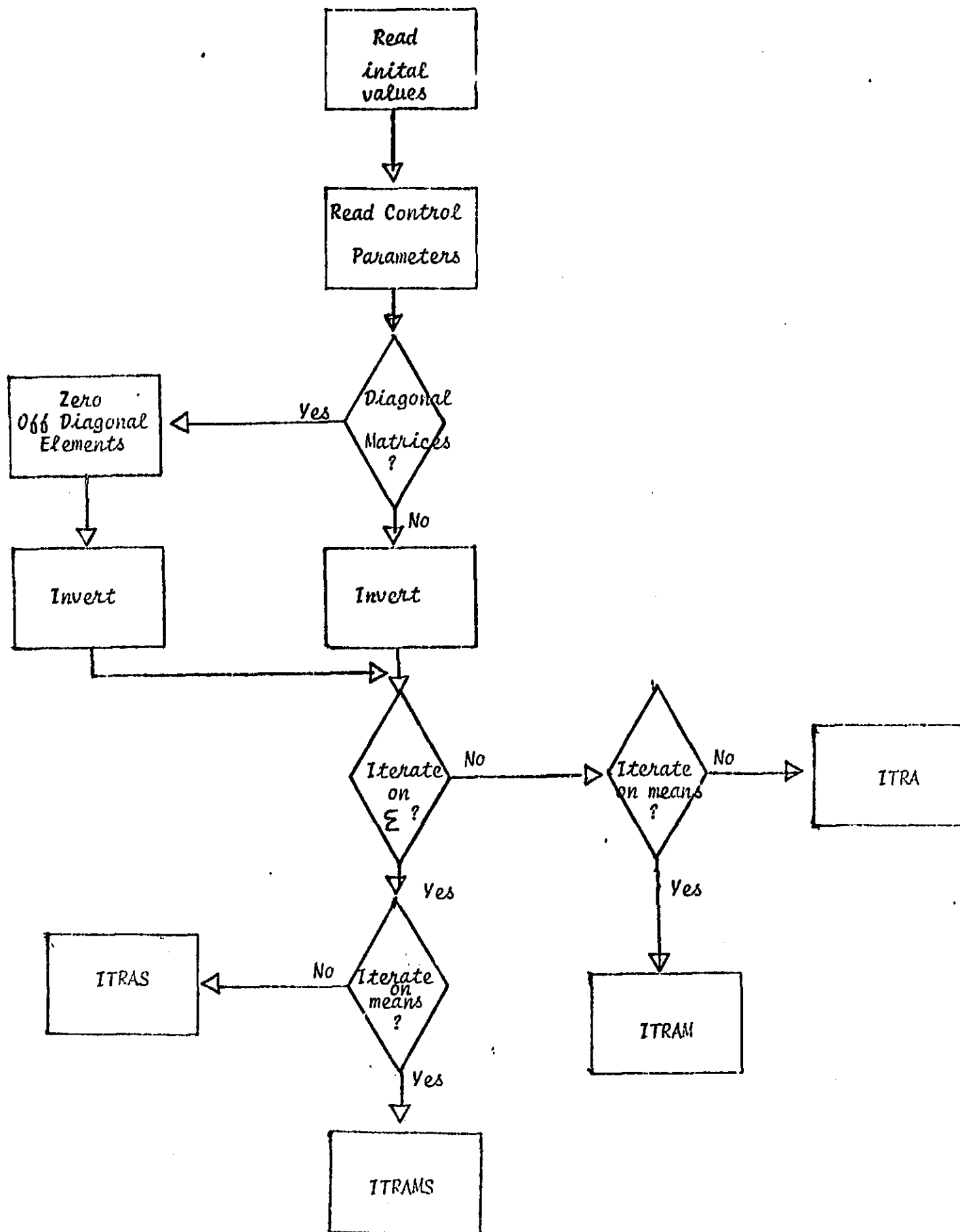
ITERATION NUMBER 2 RUN ID 'TEST'

ALPHA ,2052 ,2012 ,1939 ,1990 ,2006
DELA = ,1151414D+03

ITERATION NUMBER 0 RUN ID ITEST1

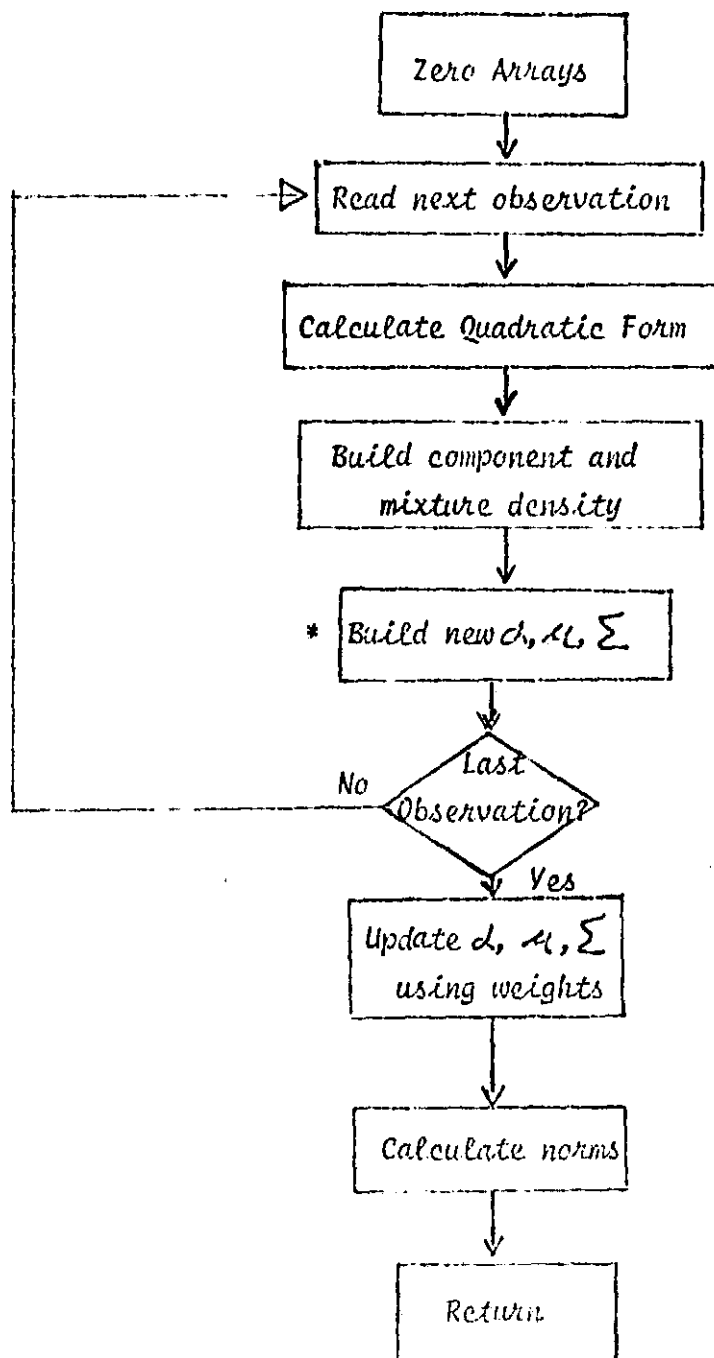
FINAL ESTIMATES PUNCHED (unit 11)

TEST	MLE OUTPUT SIGNATURES					
ALPH	.2052	.2012	.1939	.1990	.2006	
MU	16.7034	14.9441	26.1353	31.0456		
SIG	2.3907	2.9303	4.8791	.6370	.9129	1.4492
SIG	-1.3608	.8310	2.7193			.7009
MU	22.4471	25.2265	25.2865	24.6933		
SIG	.9040	.7286	1.5571	.1751	.0284	1.1312
SIG	.2184	.6583	1.0322			.1915
MU	21.1581	21.9590	29.1732	31.0526		
SIG	4.5883	8.1097	16.0956	.6068	.9891	1.0574
SIG	-4.9941	.4798	3.4870			-2.4181
MU	19.7524	21.7273	21.7716	21.1802		
SIG	.6253	.3892	1.0121	.3259	.3293	.9537
SIG	.0231	.8480	1.4683			.4382
MU	19.1637	18.0153	22.5616	23.5397		
SIG	.6039	.2613	.9172	.0578	.1689	.5851
SIG	.1715	.4705	.9680			.0143



Upon return from each subroutine the iteration tolerances are tested and when they are satisfied new control parameters are read.

FLOWCHART FOR ITRAMS



ITRAM - omits building and updating sigmas at *

ITRAS - omits building and updating means at *